1,3,5,7-Tetramethyl-2,4,6,8,9,10-hexathiaadamanta

Other names: 2,4,6,8,9,10-Hexathiaadamantane, 1,3,5,7-tetramethyl-
Tetramethylhexathiaadamantane
1,3,5,7-Tetramethyl-2,4,6,8,9,10-hexathiaadamantane
1,3,5,7-Tetramethyl-2,4,6,8,9,10-hexathioadamantane
Inchi: InChI=1S/C8H12S6/c1-5-9-6(2)12-7(3,10-5)14-8(4,11-5)13-6/h1-4H3
InchiKey: APZGKGHAXUURNO-UHFFFAOYSA-N
Formula: C8H12S6
SMILES: CC12SC3(C)SC(C)(S1)SC(C)(S2)S3
Mol. weight [g/mol]: 300.59

Physical Properties

Property code	Value	Unit	Source
hfus	6.60	kJ/mol	Joback Method
ie	8.03	eV	Cheméo Relay (1.0)
logp	5.121		Crippen Method
mcvol	189.100	ml/mol	McGowan Method
ss	321.12	J/mol×K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.24	J/mol×K	690.20	Joback Method
cpg	457.09	J/mol×K	749.86	Joback Method
cpg	474.20	J/mol×K	809.52	Joback Method
cpg	495.55	J/mol×K	869.18	Joback Method
cpg	523.15	J/mol×K	928.85	Joback Method
cpg	558.99	J/mol×K	988.51	Joback Method
cpg	605.08	J/mol×K	1048.17	Joback Method
cps	301.62	J/mol×K	298.15	NIST Webbook
hfust	23.70	kJ/mol	501.40	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6327748&Units=SI

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ss:	Solid phase molar entropy at standard conditions